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**NUMERICAL MODELING OF POLLUTANT TRANSPORT USING A
LAGRANGIAN MARKER PARTICLE TECHNIQUE**

By

Malcolm Spaulding

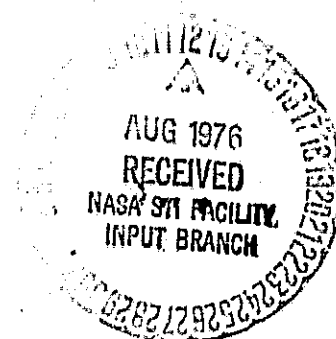
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NUMERICAL MODELING OF POLLUTANT TRANSPORT USING A LAGRANGIAN MARKER PARTICLE TECHNIQUE

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SUMMARY

A derivation and code have been developed for the three-dimensional mass transport equation, using a particle-in-cell solution technique, to solve coastal zone waste discharge problems where particles are a major component of the waste. Improvements in the particle movement techniques have been suggested and typical examples illustrated. Preliminary model comparisons with analytic solutions for an instantaneous point release in a uniform flow have shown good results in resolving the waste motion. The findings to date indicate that this computational model will provide a useful technique to study the motion of sediment, dredged spoils, and other particulate waste loads commonly deposited in coastal waters.

INTRODUCTION

The finite difference and finite element techniques have enjoyed widespread use in solving the advection-diffusion equation for water pollution transport problems. This fact is well documented in the bibliography on numerical models by Spaulding and Gordon ⁽¹⁾. In the application of these techniques to ocean waste disposal (dredged spoils or sewage sludge) and sediment transport several marked shortcomings are noted. The most serious problems encountered are: (1) generation of fictitious diffusion; (2) severe depression of concentration fields upstream of point discharges; (3) poor representation

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of constituent movement when waste consists of varying particle sizes (each with its own settling characteristics); (4) inability to readily handle resuspension of waste material on a mass dependent basis; and (5) extreme difficulty in handling scale dependent diffusion processes.

In an effort to develop a new technique which would account for these problem areas, the literature on solutions to the advective-diffusion equation was reviewed. Following recommendations made by Johnson ⁽²⁾ in a review of ocean dredge waste disposal modeling for the Corp. of Engineers and Lange et al. ^(3,4) in their work on air pollution problems, a particle-in-cell method appears particularly promising. This method has received considerable development in application to air pollution problems as noted in the work of Sklarew et al. ⁽⁵⁾, Hirt and Cook ⁽⁶⁾, and Lange et al. ^(3,4) The investigations have shown the method capable of performing useful computations to determine the fate of pollutant constituents under very complex air flow conditions.

Employing the experience gained in the air pollution field, it is felt that the particle-in-cell method provides a very useful algorithm for handling complex particulate water pollutant problems.

SYMBOLS

C	concentration of a dissolved or suspended constituent (mg/l)
t	time
\vec{U}_A	advective velocity vector ($U_A \vec{i} + V_A \vec{j} + W_A \vec{k}$)
$\vec{\nabla}$	del or gradient operator $\partial/\partial x () + \partial/\partial y () + \partial/\partial z ()$
K_{ij}	diffusivity tensor
\vec{U}_D	diffusion velocity vector ($U_D \vec{i} + V_D \vec{j} + W_D \vec{k}$)
\vec{U}_T	total pseudo transport velocity $\vec{U}_T = \vec{U}_A + \vec{U}_D$

$C_{i,j,k}$	finite difference representation of C located at $i\Delta x, j\Delta y, k\Delta z$
Δx	finite difference grid spacing in the x direction
Δy	finite difference grid spacing in the y direction
Δz	finite difference grid spacing in the z direction
x, y, z	three dimensional Cartesian coordinate axes
Δt	time increment
K_x, K_y, K_z	diagonal or principal terms of the diffusivity tensor K_{ij} in the x, y , and z directions, respectively
\vec{R}_{new}	updated position vector of a particle ($\vec{R}_{\text{new}} = \vec{x}i + y\vec{j} + z\vec{k}$) at time $t + \Delta t$
\vec{R}_{old}	previous position vector of a particle at time t
$\vec{U}_{T \text{ particle}}$	total transport velocity interpolated to the particular particle location
XP	x position of a particle within a cell referenced to the cell wall
YP	y position of a particle within a cell referenced to the cell wall
v	cell or grid volume (ΔX) (ΔY) (ΔZ)
M_i	particle mass
L	characteristic dye patch size
A_L	dissipation parameter
U_{FD}	finite difference approximation to the diffusion velocity
U_{exact}	exact differential expression for the diffusivity velocity
σ	standard deviation $\sigma^2 = \sigma_x^2 + \sigma_y^2 + \sigma_z^2$
Q	quantity of waste released
U, V, W	x, y , and z directed velocities, respectively
$\sigma_x, \sigma_y, \sigma_z$	standard deviations in the x, y , and z directions, respectively
D_{mean}	deviation of mean from the desired mean

K_α number of standard deviations for a specified confidence interval
 n number of particles
 $\sigma_{x0}, \sigma_{y0}, \sigma_{z0}$ standard deviation in the x, y , and z directions,
 respectively, at $t = 0$.

COMPUTATIONAL MODEL - WAPIC

WAPIC (water advection particle-in-cell) is a three-dimensional numerical solution code to the time dependent advection-diffusion equation for water pollutant transport employing the particle-in-cell technique. Pollutant concentration is represented statistically by embedded Lagrangian marker particles in an Eulerian grid. The discussion which follows will outline the details of the method to include its procedural steps, stability and accuracy, and program options.

Pseudo Velocity Approach

The pseudo velocity approach consists of the following. Given the transport diffusion equation

$$\frac{\partial C}{\partial t} + \vec{U}_A \cdot \vec{\nabla} C = \vec{\nabla} \cdot K_{ij} \vec{\nabla} C \quad (1)$$

where C is the concentration of the waste, K_{ij} the diffusivity tensor, and \vec{U}_A the advection velocity (from a suitable hydrodynamic model or mass consistent velocity field). Rewriting Eq. (1) in a flux conservative form with the incompressibility assumption yields:

$$\frac{\partial C}{\partial t} + \vec{\nabla} \cdot \left[C \left(\vec{U}_A - \frac{K_{ij}}{C} \vec{\nabla} C \right) \right] = 0 \quad (2)$$

If one defines a diffusion velocity as

$$\vec{U}_D = - \frac{K_{ij}}{C} \vec{\nabla} C \quad (3)$$

then a total velocity, including both the advection velocity and the diffusion velocity can be written as

$$\vec{U}_T = \vec{U}_A + \vec{U}_D \quad (4)$$

Using Eqs. (2), (3), and (4) the resulting advective-diffusion equation becomes:

$$\frac{\partial C}{\partial t} + \vec{\nabla} \cdot [C \vec{U}_T] = 0 \quad (5)$$

Equation (5) forms the fundamental starting point on which the method is based. The solution to this equation is performed in two steps: an Eulerian step and a Lagrangian step. Each will be detailed in the following paragraphs:

Eulerian Step. - From a space staggered grid system as shown in figure 1, the concentrations, C , are used to calculate the diffusivity velocities (relationship defined in Eq. (3)). A typical finite-difference representation might be

$$U_D = - \frac{2K_x}{(C_{i,j,k} + C_{i+1,j,k})} \frac{C_{i+1,j,k} - C_{i,j,k}}{\Delta x} \quad (6)$$

for the x velocity component. It has been assumed that K_{ij} reduces to K_{ii} such that $K_{11} = K_x$. In general, it is not necessary to make this approximation, however, it is commonly done. The diffusion velocities for the other coordinate directions are similarly defined as:

$$V_D = - \frac{2K_y}{(C_{i,j,k} + C_{i,j+1,k})} \frac{C_{i,j+1,k} - C_{i,j,k}}{\Delta y} \quad (7)$$

$$W_D = - \frac{2K_z}{(C_{i,j,k} + C_{i,j,k+1})} \frac{C_{i,j,k+1} - C_{i,j,k}}{\Delta z} \quad (8)$$

with these difference approximations the diffusion velocities are seen to be defined at the same points in the grid system as the advective velocities. This scheme proves to be very useful when calculating the total velocity at any position in the grid system.

The final task to be performed in this step of the computation is the addition of the advective and diffusion velocities to determine the total or pseudo transport velocity. Since both velocities have been defined at the same location in the grid system, a simple addition for each coordinate direction velocity is all that is required.

Lagrangian Step.- Each marker particle contained in an Eulerian cell is transported for one time step Δt according to the total transport velocity U_T (defined in Eq. (4))

$$\vec{R}_{\text{new}} = \vec{R}_{\text{old}} + \vec{U}_{T \text{ particle}} \Delta t \quad (9)$$

where \vec{R}_{old} is the Lagrangian particle position at time step t , \vec{R}_{new} is the position at time step $t + \Delta t$ and $\vec{U}_{T \text{ particle}}$ is the bilinear weighted velocity at the particle for time step t . Figure 2 shows a simple two-dimensional example for determining the velocities at a particular particle location. This approach can readily be generalized to the three-dimensional case.

Although the bilinear weighting scheme or a slight variation has been used to determine the velocity at particle locations in the models of Lange and Knox ⁽⁴⁾ for the air pollutant transport problems, it is felt that this technique is not adequate. In particular, when the streamlines or pathlines of the flow field are curved, the marker particles tend to drift in such a manner that the true streamlines and those given by the marker particles are not coincident. By reducing the time step Δt the error can be reduced substantially; however, at the expense of computational time and, therefore, cost.

Forester ⁽⁷⁾ has proposed an iterative approach to particle motion prediction that alleviates many of the problems inherent with the simple bilinear velocity weighting scheme. Instead of employing Eq. (9) to represent

the particle motion computation, he suggests the following:

$$\vec{R}_{\text{new}} = \vec{R}_{\text{old}} + \left(\vec{U}_{T \text{ particle}}^{\text{old}} + \vec{U}_{T \text{ particle}}^{\text{new}} \right) \frac{\Delta t}{2} \quad (10)$$

where $\vec{U}_{T \text{ particle}}^{\text{old}}$ represents the bilinear weighted velocity at the old particle position \vec{R}_{old} and $\vec{U}_{T \text{ particle}}^{\text{new}}$ represents the bilinear weighted velocity at the new particle position \vec{R}_{new} . With an iteration procedure where each estimate of \vec{R}_{new} is used to calculate an updated particle velocity $\vec{U}_{T \text{ particle}}^{\text{new}}$ Eq. (10) is solved to find the new particle positions, for a given convergence error on \vec{R}_{new} .

In an attempt to assess the usefulness of the iteration procedure, several trial cases have been executed. Using a simple four-cell velocity field with rotational currents (as shown in figures 3 and 4), a grid spacing of 10 m in both the x and y directions, and varying time step, particle trajectories were predicted with and without the iteration procedure previously outlined. Figure 3 shows that without iteration and even for very small time steps (i.e., 1/10 of a grid space per time step) the trajectories show a definite spiraling outward from the true particle pathline--a closed circle for this velocity field. Figure 4 presents the same simulations but employing the iteration procedure. It is readily seen that there is a marked improvement in particle trajectory representation with this approach.

Therefore, it is concluded that the use of the proposed iteration technique is the best method to determine particle motion, since it requires less computational effort for more accurate results. Without this procedure, it can be seen that eddy type structures are more rapidly depleted of their pollutant loads than occurs in the real case.

The final portion of the Lagrangian step is to compute the concentration given the new particle positions and mass. A "fictitious" volume is associated

with each particle mass at the start of the computation. The overlap of this volume into the surrounding Eulerian cells determines the distribution of mass into the various cells and allows the concentration field to be calculated. Figure 5 shows the details of the computational procedure for a typical particle in a two-dimensional grid system. This algorithm is simply repeated for all particles in the system for a given time. A further refinement can be added in the Lagrangian step to allow for grid expansion or a grid system that moves with the mean motion of the particles. Incorporation of this feature permits maximum resolution of the concentration field with a minimum number of computational grids, and is particularly useful for determining the behavior of "puff" or instantaneous point releases. Variations of the moving grid system procedure would allow the resolution of some particular portion of the pollutant field, i.e., determining where particles of a specified mass are transported.

Figure 6 presents a flow chart for the computational procedure that has been outlined in the previous paragraphs.

Velocity Information

In order to perform computations with WAPIC, a mass consistent velocity field is required. That is a velocity field that conserves water mass. This information for both spatial and temporal variations can be obtained from a finite difference or finite element model of the coastal zone hydrodynamics. Reference 1 gives an extensive list of suitable circulation models of both the two-dimensional vertically averaged and three-dimensional types. It is also possible to use statistical predictor type models (8,9) based on data taken for a particular area. The main requirement of each, however, is conservation of water mass.

The final requirement of the flow field is that the velocity information can be resolved into the space staggered grid system as shown in figure 1. A simple linear weight processing technique with a water conservation constraint should readily achieve this goal.

Boundary Conditions

WAPIC has two basic types of boundary conditions, a closed or zero mass flux boundary ($\vec{U}_T \text{ particles } C = 0$), and a mass flux boundary ($\vec{U}_T \text{ particles } C = \text{constant}$). In the application of these boundary specifications, consistency of boundary type for both the Eulerian and Lagrangian step calculations as well as the input velocity field must be maintained. Specifically, the Eulerian step must account for the flux of pollutant particles due to diffusion while the Lagrangian step resolves the advective particle flux.

Another boundary condition particularly applicable to the sediment transport problem is a deposition or storage boundary. When particles which are settling from the flow field reach the bottom of the water column they may be stored at that geographic location until such time as they might be resuspended by an increased shear at the water-soil interface.

Diffusion Parameters

In the general case, WAPIC can, in principle, accommodate the full Cartesian eddy diffusivity tensor K_{ij} . In practice, isotropy of the water turbulence is assumed and only the diagonal terms noted as K_x , K_y , and K_z remain. In addition, for most coastal zone flow conditions it is generally assumed $K_x \approx K_y$. It still remains, however, to determine values or empirical relations that approximate the diffusion processes for coastal zone areas.

The majority of investigations for horizontal turbulent diffusion in the ocean monitor the size of tracer dye patch as a function of time and then using simple diffusion models, which disregard both shear current and vertical transport, calculate the diffusion coefficients (10).

The values of horizontal diffusion coefficients obtained in the ocean range from 5×10^2 to 4×10^8 cm²/sec. The largest number of measurements were obtained at the ocean surface. In general, it was found that the K_x was a direct function of the diffusing patch size L . Figure 7 shows a collection of data and illustrates this relationship quite well. Although the data scatter is significant, in general

$$K_x \approx A_L L^{4/3} \quad 10^{-1} \text{ ft} \leq L \leq 10^8 \text{ ft} \quad (11)$$

where A_L is a constant called the dissipation parameter and varies from 0.005 to 0.00015 ft^{2/3}/sec.

Diffusion coefficients obtained in the ocean are not strictly applicable to estuarine waters; they are, however, useful in demonstrating trends and magnitudes. Brandsma and Dlvoky (12) have shown that data from tidal estuaries lie right on the ocean data when applying the four-thirds power law. Therefore, Eq. (11) should be a useful first approximation to horizontal diffusion parameters for both coastal zone and estuarine waters. Further refinements to horizontal diffusion prediction will probably rely on field experiments in the local area.

The vertical diffusion coefficient in the ocean is generally much smaller than the horizontal coefficient. Table I shows a summary of typical values employed for a variety of coastal and open ocean conditions. Although there appear to be no general relations for vertical diffusion, it normally displays a maximum near the surface (caused by wind mixing) and decreases with depth.

In addition, the vertical mixing decreases as the Richardson number (measure of density stratification) increases. Table II indicates some typical formulations for the vertical diffusion coefficient.

Accuracy and Stability Requirements

In all numerical solutions to the advective-diffusion transport equations, there are requirements which must be met in order to achieve accurate and stable solutions to the equations. Discussed below are detailed conditions for the pseudo velocity approach.

Number of Eulerian Cells per Problem. - It is a basic requirement for all methods that use Eulerian grid systems and finite difference or elements approximations that sufficient grids are used to resolve the concentration gradients of interest. When this condition is achieved, the numerically calculated gradients of concentration and the actual gradients agree with one another. In addition, as the cells used to represent the concentration field increase the agreement between actual concentrations and those of the numerical computation becomes better.

In an effort to develop an approximate quantitative estimate of the lower limit and the number of grids necessary to resolve the concentration distribution, we will follow the approach outlined by Lange ⁽³⁾. Consider the one-dimensional finite difference approximation to the diffusion velocity given by:

$$U_{i+1/2} = - \frac{K_{x_{i+1/2}}}{\Delta x} \frac{(C_{i+1} - C_i)}{C_{i+1/2}} \quad (12)$$

Using a Taylor series expansion about $i + 1/2$ for C_{i+1} and C_i , substituting into Eq. 12 and dropping the $i + 1/2$ subscript yields

$$U = - \frac{K_x}{\Delta x C} \left[\frac{\partial C}{\partial x} \Delta x + \frac{1}{24} \frac{\partial^3 C}{\partial x^3} \Delta x^3 + \text{higher order terms} \right] \quad (13)$$

Then expanding Eq. (13) and dropping higher order terms gives

$$U = - \frac{K_x}{C} \frac{\partial C}{\partial x} - \frac{K_x}{24} \frac{\Delta x^2}{C} \frac{\partial^3 C}{\partial x^3} \quad (14)$$

The first term on the right-hand side of Eq. (14) is the exact differential expression for the diffusivity velocity. Taking the ratio of the diffusion velocity defined by finite differences (Eq. (14)) and the exact differential results in:

$$\frac{U_{FD}}{U_{exact}} = 1 + \frac{\frac{\partial^3 C}{\partial x^3}}{\frac{\partial C}{\partial x}} \frac{\Delta x^2}{24} \quad (15)$$

In order to obtain a quantitative measure of this ratio estimates of the first and third derivatives of concentration with distance are required.

Assuming a simple one-dimensional Gaussian distribution:

$$C = \frac{Q}{\sigma} e^{-x^2/2\sigma^2} \quad (16)$$

and finding the first

$$\frac{\partial C}{\partial x} = - \frac{Qx}{\sigma^3} e^{-x^2/2\sigma^2} \quad (17)$$

and third derivatives

$$\frac{\partial^3 C}{\partial x^3} = \frac{Qx}{\sigma^5} \left[3 - \frac{x^2}{\sigma^2} \right] e^{-x^2/2\sigma^2} \quad (18)$$

this estimate can be made.

Substituting Eqs. (17) and (18) into Eq. (15) one obtains

$$\frac{U_{FD}}{U_{exact}} = 1 - \frac{1}{24} \left(\frac{x^2}{\sigma^2} - 3 \right) \frac{\Delta x^2}{\sigma^2} \quad (19)$$

Employing the fact that 99.9 percent of all particles in a one-dimensional

Gaussian distribution are within $x = 3\sigma$, we can substitute $x = 3\sigma$ in Eq. (19) and find

$$\frac{U_{FD}}{U_{exact}} = 1 - \frac{\Delta x^2}{4\sigma^2} \quad (20)$$

From this relationship, it is seen that when a grid cell is either larger or comparable to the standard deviation for particle distribution, the finite difference algorithm underestimates the diffusion velocity. However, as more grid cells are employed for a given standard deviation, the finite difference approximation becomes an increasingly better estimate of the diffusion velocity.

Number of Particles per Cell.- Since the particles represent a statistically quantized density, it is desirable to have as many particles as possible for any particular problem. An upper bound on particles would be either the storage capability or maximum program run time (this is directly proportional to the number of particles) for a particular computer. The lower bound is at least one particle per cell. Fewer particles and in particular when a particle has no neighbors within one cell length, the particle is moved to the grid boundary and "frozen" in place when considering the diffusion velocity. This freezing process is a direct consequence of the algorithm for determining concentrations from particle positions (see figure 5). It can be readily seen that any particle must distribute its mass to its nearest neighbor cells. If another distribution algorithm were chosen which distributed the particles over a greater volume, the one particle per cell minimum could be relaxed.

Particle Generation.- In general, it is desirable to start either steady state or time dependent point discharge simulations with some initial Gaussian or normal distribution. Several experiments were conducted using random number generator techniques similar to those in the work of Lange ⁽³⁾, which proved

to give distributions that displayed noticeable "bunching" of particles around the directions of the coordinate axes. It was felt that this problem was directly related to the quality of the normal random number generator available at the time.

In an effort to alleviate this problem, it was decided to specify the exact number of particles in each cell using the Gaussian probability distribution function. Knowing the cell size, standard deviation of the distribution, and the total number of particles in the field one can then compute the number of particles in each cell using the normal distribution constraint. Next, a uniform random number generator was used to locate the appropriate number of particles in each cell. All cells were filled in this manner. If it is decided to obtain another type of initial condition, all one needs to do is specify the desired distribution as a constraint for defining the manner in which these cells are to be filled with particles. The remainder of the algorithm remains unchanged.

Time Step Restriction. - Similar to many finite difference schemes, WAPIC has a restriction that the fastest moving particle cannot move more than one-half cell length in one time step, Δt . In equation form this restriction becomes

$$\text{maximum} \left[\frac{U_T \Delta t}{\Delta x}, \frac{V_T \Delta t}{\Delta y}, \frac{W_T \Delta t}{\Delta z} \right] \leq 1/2 \quad (21)$$

where U_T , V_T , and W_T are the total or pseudo transport velocities Δt is the time step, and Δx , Δy , and Δz are the grid spacings in the x, y, and z directions, respectively. These are accuracy conditions rather than stability ones.

As was discussed earlier, if one does not choose to employ the iteration particle location technique and the flow-field displays marked eddy structure

or curved streamlines, it becomes necessary to further restrict the maximum time step. The exact value to be employed in that particular situation is highly problem dependent and it is, therefore, recommended to use the iteration procedure in all cases.

Number of Particles for Given Confidence Limit on Mean. - When undertaking a problem, it is extremely desirable to have at least a first estimate of the number of particles necessary to define a particular distribution or starting condition. Since the Gaussian distribution is often employed to define the initial conditions, a logical manner to determine the number of particles is to use simple statistical theory to find the number of particles necessary to assume a given confidence in the deviation of the mean from the desired mean.

In Bowker and Lieberman's text (13) it is shown that the lower one-sided deviation from the mean confidence limit is:

$$D_{\text{mean}} = K_{\alpha} \frac{(\sigma_x^2 + \sigma_y^2 + \sigma_z^2)^{1/2}}{\sqrt{n}}$$

$$\sigma^2 = \sigma_x^2 + \sigma_y^2 + \sigma_z^2$$

where D_{mean} - deviation of the mean from the desired value, σ - the standard deviation of the normal distribution, n - the number of particles, and K_{α} - the number of standard deviations for a given confidence interval (e.g., for 95 percent confidence interval $\sim K_{\alpha} = 1.645$).

In an effort to gain a more quantitative estimate of this relation, a parametric study on confidence limit (70 - 95 percent) with a $\sigma_x = \sigma_y = 1000$ m, $\sigma_z = 1.5$ m, and a mean of 5000 m is shown in figure 8. In general, it indicates that for this distribution about 1000 particles are adequate to define the initial conditions.

The influence of σ on the number of particles for a given confidence limit and deviation from the mean is shown in figure 9. As expected the

smaller the standard deviation the less particles necessary to define the mean to within a given confidence interval.

Although figures 8 and 9 are for a particular problem, the technique outlined provides a simple procedure to determine an order of magnitude estimate of the number of particles necessary for a given problem. In addition, preliminary estimates on error bounds for subsequent program solution can be obtained.

Options in WAPIC

Sources and Sinks.- Sources or sinks of pollutant can be generated anywhere within the Eulerian grid mesh and may either be instantaneous, continuous, or intermittent. From accuracy considerations, previously discussed, the initial pollutant distribution must cover at least two grid lengths, otherwise, the particles diffuse too slowly. This, therefore, requires special sub-grid treatment if accurate near-field results are necessary.

Deposition and Resuspension.- The deposition of particles can readily be accommodated with WAPIC. Knowing the particle density and shape/surface characteristics, a settling velocity can be approximated for each particle and simply added to the total transport velocity. The ability to handle each particle separately allows highly detailed behavior of waste material containing varying size distribution such as sediment or dredged material to be predicted.

Resuspension of material from the bottom or some other storage area can be handled on a particle size basis provided the hydrodynamic model input provides sufficient detail of bottom current structure.

Flocculation.- A rather prevalent process in the settling of fine sediment and waste material is flocculation. Electrostatic forces between neighboring

particles cause an aggregate to be formed with new settling characteristics. Classical finite difference and finite element solutions to the advective-diffusion equation are unable to represent this process very accurately since they rely on a gross adjustment, such as an additional sink of the waste material to replicate the flocculation process.

WAPIC allows one to assign electrostatic and other properties to a given particle and the separation distance between particles is easily obtained from the Lagrangian marker paths. With this information, better resolution of the details of flocculation can be achieved.

Time History of Particles.- In some sediment transport studies, radioactive tracer materials are used to monitor the time dependent sediment motion. Using the detailed time history of the particles available with WAPIC, one can assume given radioactive decay rates for the tracer particles as they travel along their trajectories. These time path histories, therefore, provide an additional capability over classical solutions to the advective-diffusion equation.

VERIFICATION

In an effort to perform preliminary model verification, several simple instantaneous releases of pollutant were simulated. A spherically symmetric Gaussian puff distribution consisting of 1984 particles was instantaneously released into a uniform velocity field. The model parameters for this case were:

Grid spacing $\Delta x = \Delta y = 500 \text{ m}$ $\Delta z = 1.5 \text{ m}$

Diffusion Coefficients $K_x = K_y = 10 \text{ m}^2/\text{sec.}$, $K_z = 0.0001 \text{ m}^2/\text{sec.}$

Standard Deviations

(of initial distributions) $\sigma_{x0} = \sigma_{y0} = 1000 \text{ m}, \sigma_{z0} = 1.5 \text{ m}$

Time step $\Delta t = 250 \text{ sec.}$

Grid system with mean particle motion.

A corresponding analytical solution for this problem was obtained from the work of Kubo et al. (14) and modified to include an initial distribution of the concentration field. The solution is given by

$$C(x,y,z,t) = \frac{G}{(2\pi)^{3/2} \left(\sigma_{x0}^2 + 2K_x t \right)^{1/2} \left(\sigma_{y0}^2 + 2K_y t \right)^{1/2} \left(\sigma_{z0}^2 + 2K_z t \right)^{1/2}} \times \exp \left[-\frac{1}{2} \left(\frac{(x - ut)^2}{\sigma_{x0}^2 + 2K_x t} + \frac{y^2}{\sigma_{y0}^2 + 2K_y t} + \frac{z^2}{\sigma_{z0}^2 + 2K_z t} \right) \right] \quad (23)$$

Comparison of the model results with the analytic solution are shown in figures 10 and 11. Figure 10 gives a comparison of the concentration distribution in downstream direction for several time increments. Only half of the profiles were plotted on the first and last time steps in order to aid in interpreting the graph. The variation of model predictions to data is with ± 5 percent for all cases. Figure 11 shows a similar graph but in the vertical plane. Again, the comparison appears within 5 percent. If an increased number of particles were employed and better initial resolution (finer than $\sigma_{x0} = \sigma_{y0} = 2\Delta x, \sigma_{z0} = \Delta z$) this error in model predictions could be further reduced.

CONCLUSIONS

A derivation and code have been developed for the three-dimensional mass transport equation, using a particle-in-cell solution technique, to solve coastal zone waste discharge problems where particles are a major component of the waste. Improvements in the particle movement techniques have been

suggested and typical examples illustrated. Preliminary model comparisons with analytic solutions for an instantaneous point release in a uniform flow have shown good results in resolving the waste motion. The findings to date indicate that this computational model will provide a useful technique to study the motion of sediment, dredged spoils, and other particulate waste loads commonly deposited in coastal waters.

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TABLE I

SUMMARY OF VALUES
OF VERTICAL DIFFUSION COEFFICIENT K_z IN THE OCEAN
(Reference 10)

Note: Molecular diffusivity for heat: $1.5 \times 10^{-3} \text{ cm}^2/\text{sec}$ (at 20°C , 1 atm)
salt: $1.3 \times 10^{-5} \text{ cm}^2/\text{sec}$ (at 20°C , 1 atm)

Current or oceanic region	Depth of layer (m)	Vertical Diffusion Coefficient K_z (cm^2/sec) ²	Reference
Philippine Trench	5000-9788	2.0-3.2	Schmidt, 1917
Algerian Coast	0- 20	35-40	Schmidt, 1917
Mediterranean	0- 28	42	Schmidt, 1917
California Current	0- 200	30-40	McEwen, 1919
Caspian Sea	0- 100	1-3	Stockman, 1936
Barents Sea	-----	4-14	Subov, 1938
Bay of Biscay	0- 100	2-16	Fjeldstad, 1933
Equatorial Atlantic Ocean	0- 50	320	Defant, 1932
Randesfjord	0- 15	0.1-0.4	Jacobsen, 1913
Schultz Grund	0- 25	0.04-0.74	Jacobsen, 1913
Kuroshio	0- 200	30-80	Sverdrup-Staff, 1942
Kuroshio	0- 400	7-90	Suda, 1936
Southern Atlantic Ocean	400-1400	5-10	Defant, 1936
Arctic Ocean	200- 500	20-50	Sverdrup, 1933
Carribean Sea	500- 700	2.8	Seiwell, 1938
South Atlantic Ocean	3000-Bottom	4	Defant, 1936
South Atlantic Ocean	Near Bottom	4	Wattenberg, 1935
West Atlantic Trough (50°S to 10°N)	Near Bottom	7-50	Wüst, 1955
North Atlantic			
Indian Ocean			
Pacific Ocean	Near Bottom	4-30	Koczy, 1956
Tidal Channel (Mersey estuary and Irish Sea)	0- 20 (bottom)	2-40	Bowden, 1965 (with R_1 from 0.1 to 2.0)
Near Cape Kennedy, Florida	Surface Layer	19 (in August) 1.3 (in Summer)	Carter and Okubo, 1965
Bikini Lagoon	0- 50 (bottom)	260	Munk, Ewing and Revelle, 1949
Coast of Denmark		0.05-1	Harremoes, 1967
California Coast		0.1-10	Foxworthy, Tibbels, and Barsom, 1966
-----	4	15-180 (at wind force 3-4)	Stommel and Woodcock, 1951

* As given by Defant, 1961

** As given by Bowden, 1962

*** As given by Harremoes, 1967

**** As given by Wiegell, 1964

TABLE 11

SUMMARY OF FORMULAS
ON CORRELATION OF VERTICAL DIFFUSION COEFFICIENT K_z
WITH RICHARDSON'S NUMBER R_i (OR DENSITY GRADIENT ϵ)
(Reference 10)

Note: $K_{z0} : K_z$ at $R_i = 0$, i.e., the neutral case θ : proportionality constant varies from case to case

Rossby and Montgomery (1935)*	$K_z = K_{z0} (1 + \theta R_i)^{-1}$	
Rossby and Montgomery (1935)*	$K_z = K_{z0} (1 + \theta R_i)^{-2}$	
Holzman (1943)*	$K_z = K_{z0} (1 - \theta R_i)$	$R_i \leq \frac{1}{\theta}$
Yamamoto (1959)*	$K_z = K_{z0} (1 - \theta R_i)^{1/2}$	$R_i \leq \frac{1}{\theta}$
Mamayev (1958)*	$K_z = K_{z0} e^{-\theta R_i}$	
Munk and Anderson (1948)**	$K_z = K_{z0} (1 + \theta R_i)^{-3/2}$ $\theta = 3.33$ based upon data by Jacobsen (1913) and Taylor (1931)	
Harremoes (1968)	$K_z = 5 \times 10^{-3} \times \epsilon^{-2/3} \text{ cm}^2/\text{sec}$ note: ϵ in m^{-1} ; approximate experimental range $5 \times 10^{-9} < \epsilon < 15 \times 10^{-5} \text{ m}^{-1}$	
Kolesnikov, et al (1961)***	$K_z = K_{z \text{ min}} + \frac{\theta}{\epsilon} \ln \text{ cm}^2/\text{sec}$ $K_{z \text{ min}}$ and θ are empirically determined to be: $K_{z \text{ min}} = 12, \theta = 8.3 \times 10^{-5}$ (1958 and 1960 observations) $K_{z \text{ min}} = 2, \theta = 10.0 \times 10^{-5}$ (1959 observations)	
Koh and Fan (1969)	$K_z = 10^{-4}/\epsilon$ (K_z in cm^2/sec ; ϵ in m^{-1}) $4 \times 10^{-7} \leq \epsilon \leq 10^{-2} \text{ m}^{-1}$	

* As given by Okubo (1962)

** As given by Bowden (1962)

*** The formulas presented in the translated version are apparently erroneous.

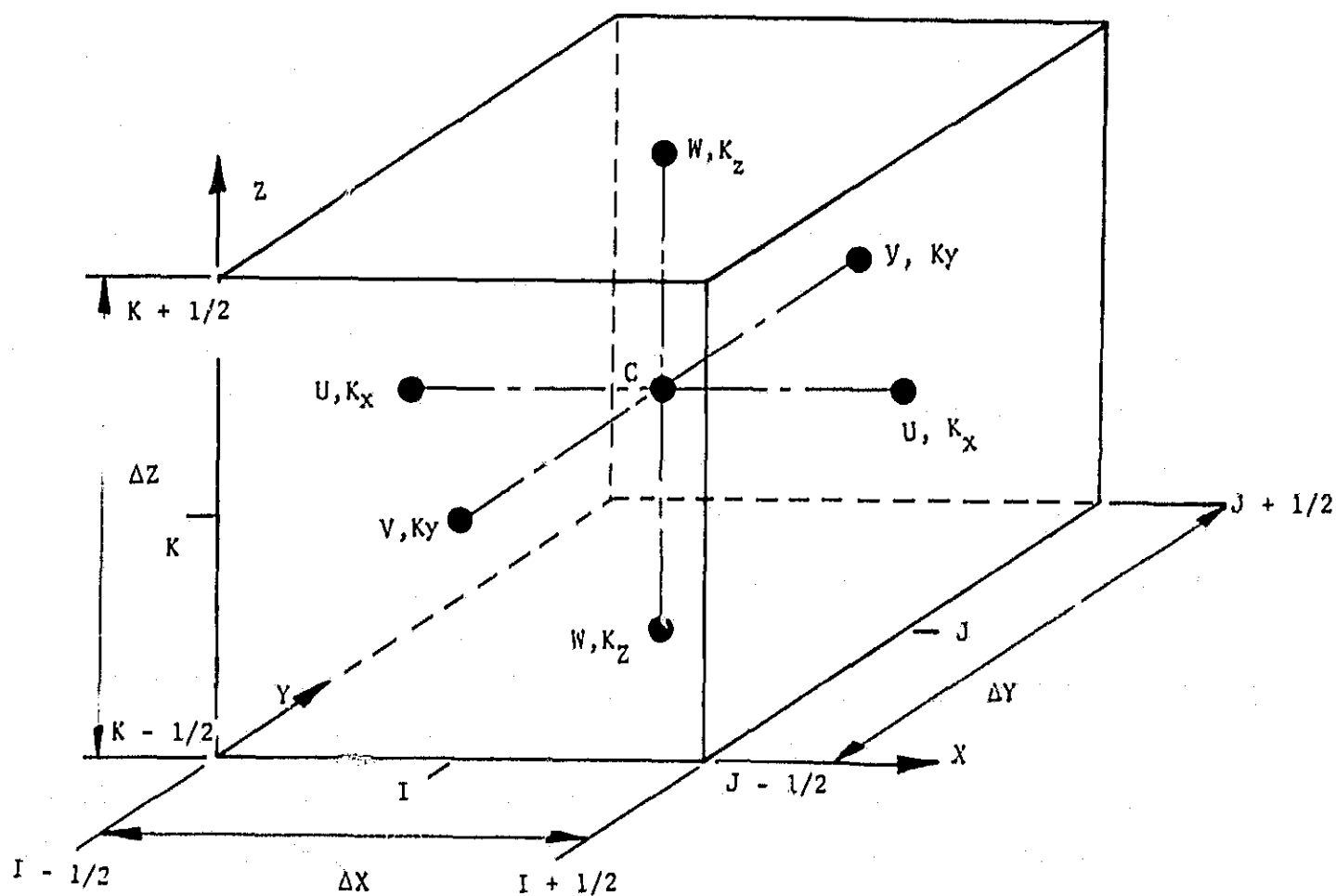
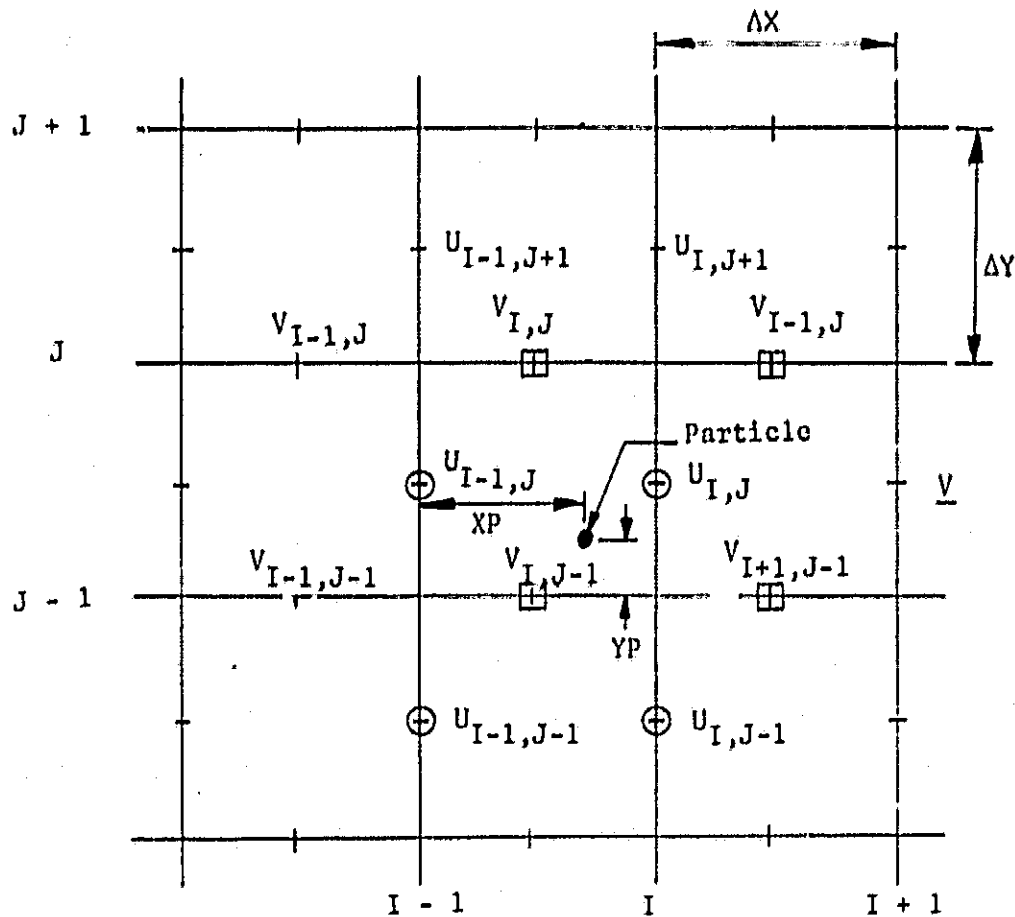


Figure 1.- Three Dimensional Space Staggered Grid System



X DIRECTED VELOCITY (U_p) AT PARTICLE POSITION

$$U_1 = \frac{XP}{\Delta X} (U_{I,J} - U_{I-1,J}) + U_{I-1,J}$$

$$U_2 = \frac{XP}{\Delta X} (U_{I,J-1} - U_{I-1,J-1}) + U_{I-1,J-1}$$

$$U_p = \frac{(YP + \Delta Y/2)}{\Delta Y} (U_1 - U_2) + U_2$$

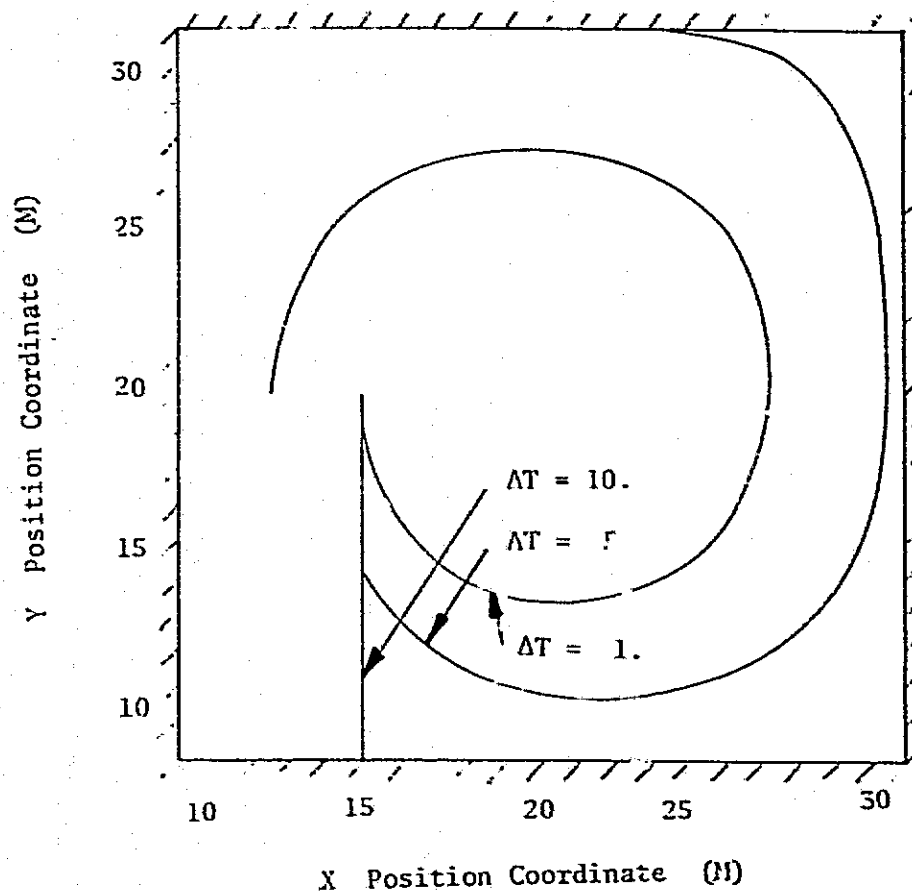
Y DIRECTED VELOCITY (V_p) AT PARTICLE POSITION

$$V_1 = \frac{YP}{\Delta Y} (V_{I,J} - V_{I,J-1}) + V_{I,J-1}$$

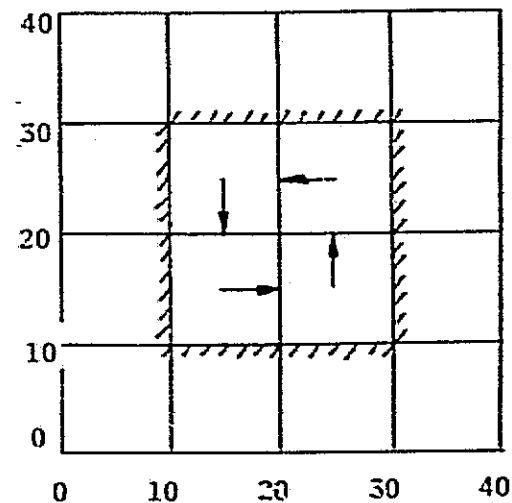
$$V_2 = \frac{YP}{\Delta Y} (V_{I+1,J} - V_{I+1,J-1}) + V_{I+1,J-1}$$

$$V_p = \frac{(XP - \Delta X/2)}{\Delta X} (V_2 - V_1) + V_1$$

Figure 2.- Simple Two Dimensional (X,Y) Relations
To Determine the Bilinear Velocities
At The particle Positions.

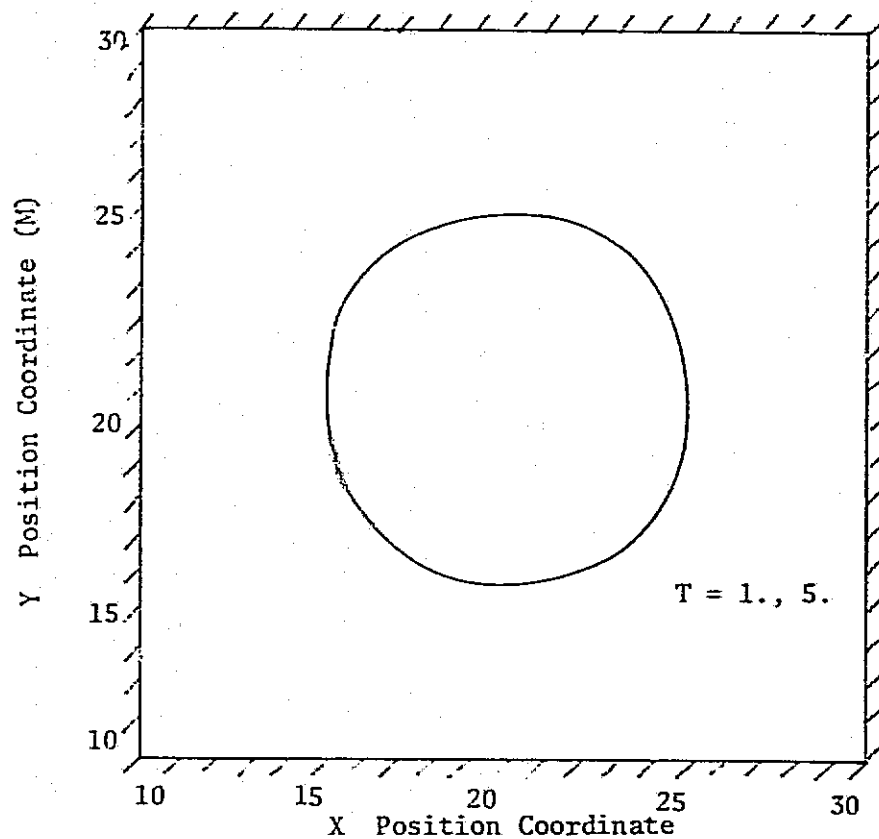


Velocity - 1 M/Sec.
 Grid Spacing
 $\Delta X = 10M$
 $\Delta Y = 10M$
 Time Step $\Delta t = 1, 5, \text{ \& } 10 \text{ Sec.}$



Grid System Showing Velocity Field

Figure 3.- Particle Trajectories for Varying Time Steps (1,5, and 10 Sec.) Without Position Iteration.



Velocity - 1 M/sec.

Grid Spacing

X ΔX - 10 M

Y ΔY - 10 M

Time Step ΔT - 1, and 5 Sec.

Convergence Error - .01

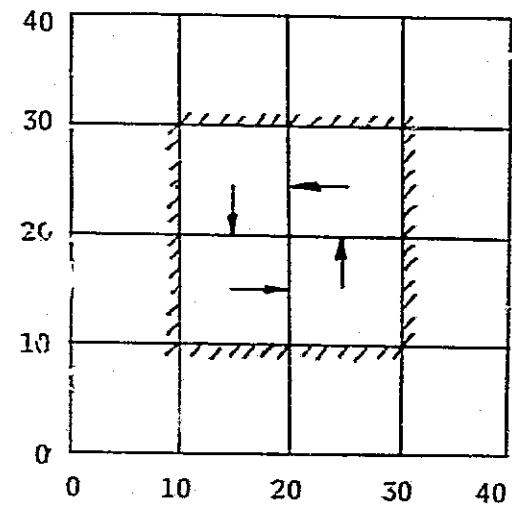
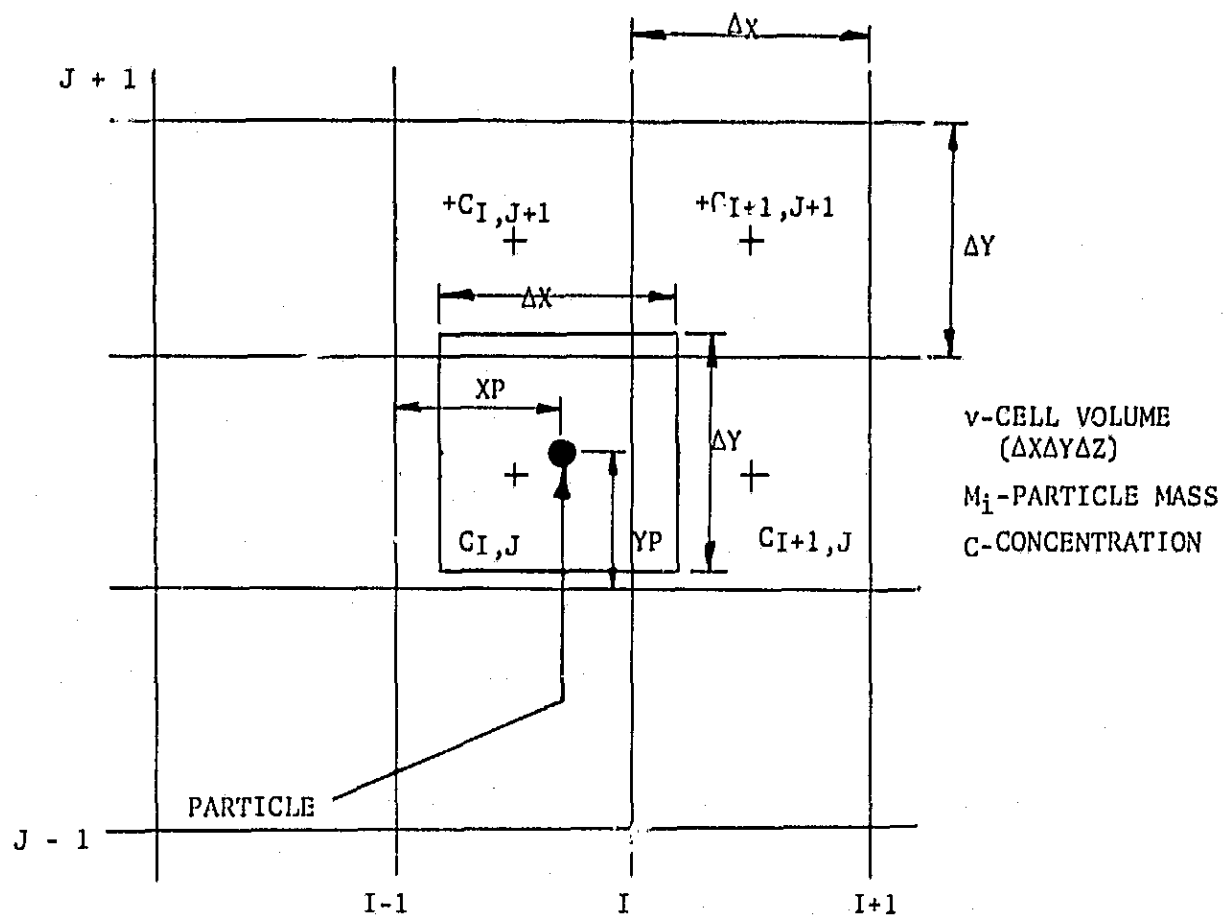


Figure 4. - Particle Trajectories for Varying Time Steps (1 and 5 Sec.) with Position Iteration.



CONCENTRATION COMPUTATIONS

$$C_{I,J} = \frac{M}{V^2} (\Delta Z) \left(\frac{3\Delta X}{2} - XP \right) \left(\frac{3\Delta Y}{2} - YP \right)$$

$$C_{I+1,J} = \frac{M}{V^2} (\Delta Z) \left(XP - \frac{\Delta X}{2} \right) \left(\frac{3\Delta Y}{2} - YP \right)$$

$$C_{I+1,J+1} = \frac{M}{V^2} (\Delta Z) \left(XP - \frac{\Delta X}{2} \right) \left(YP - \frac{\Delta Y}{2} \right)$$

$$C_{I,J+1} = \frac{M}{V^2} (\Delta Z) \left(\frac{3\Delta X}{2} - XP \right) \left(YP - \frac{\Delta Y}{2} \right)$$

Figure 5.- Computational Algorithm to Determine Concentrations, given Particle Position and Mass.

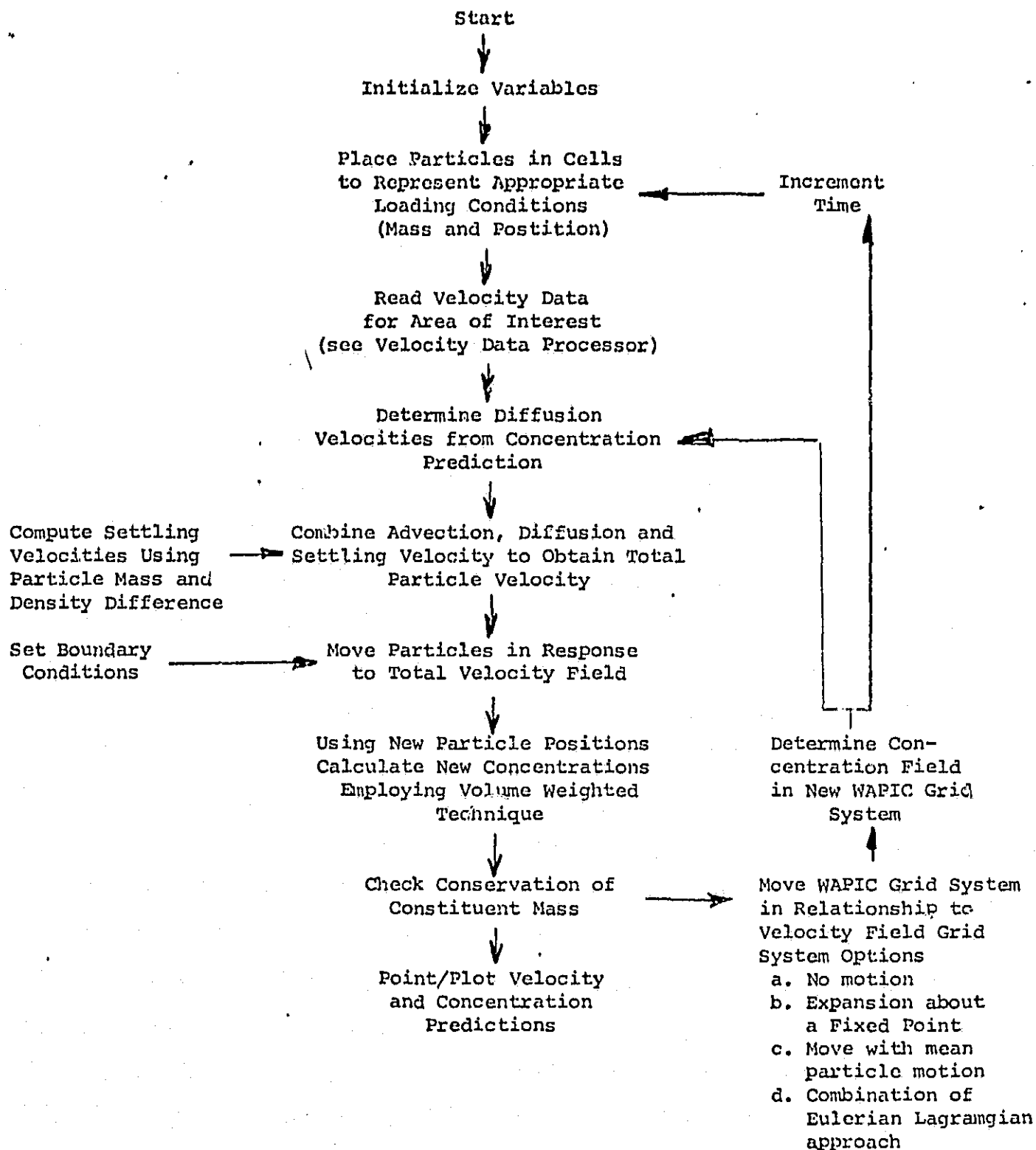


FIGURE 6 Generalized Flow Chart for WAPIC

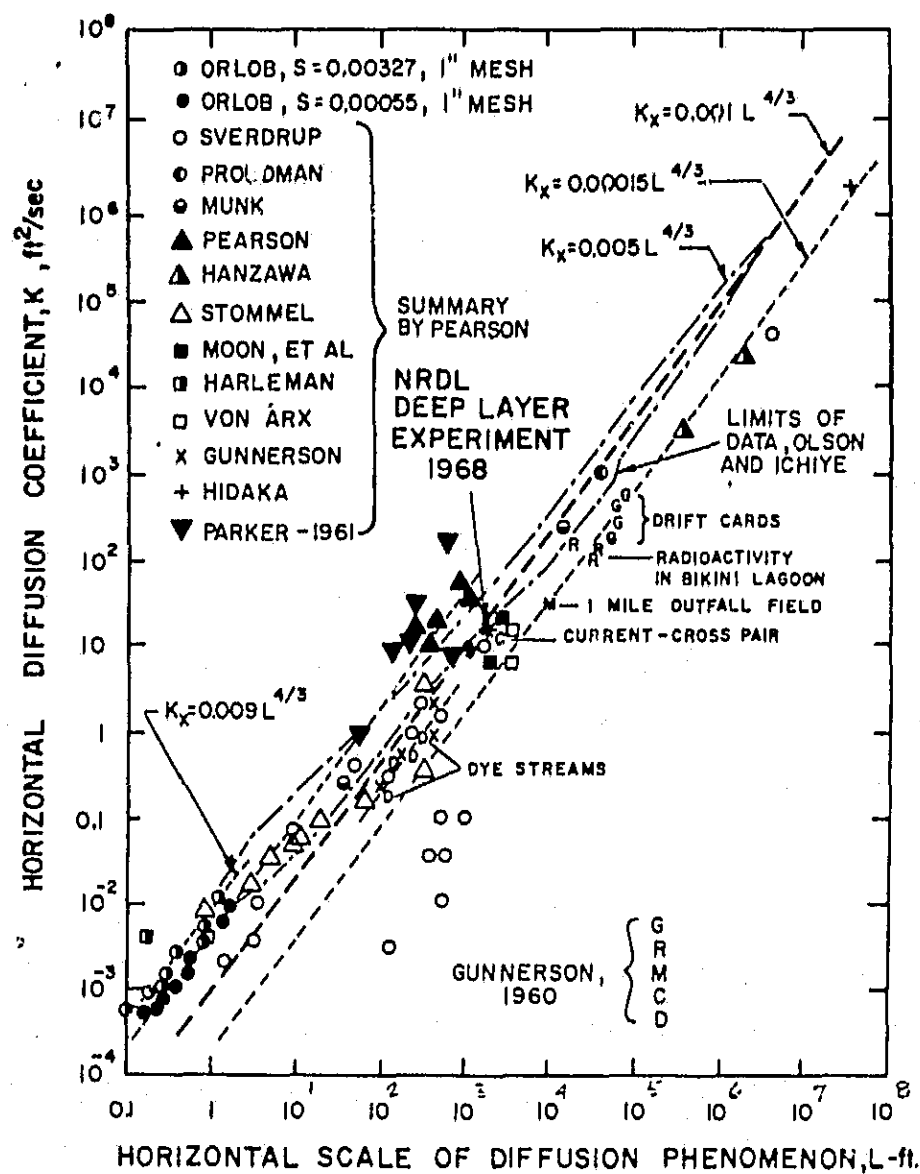


Figure 7. Horizontal Diffusion Coefficient as a function of Horizontal Scale (Reference 11)

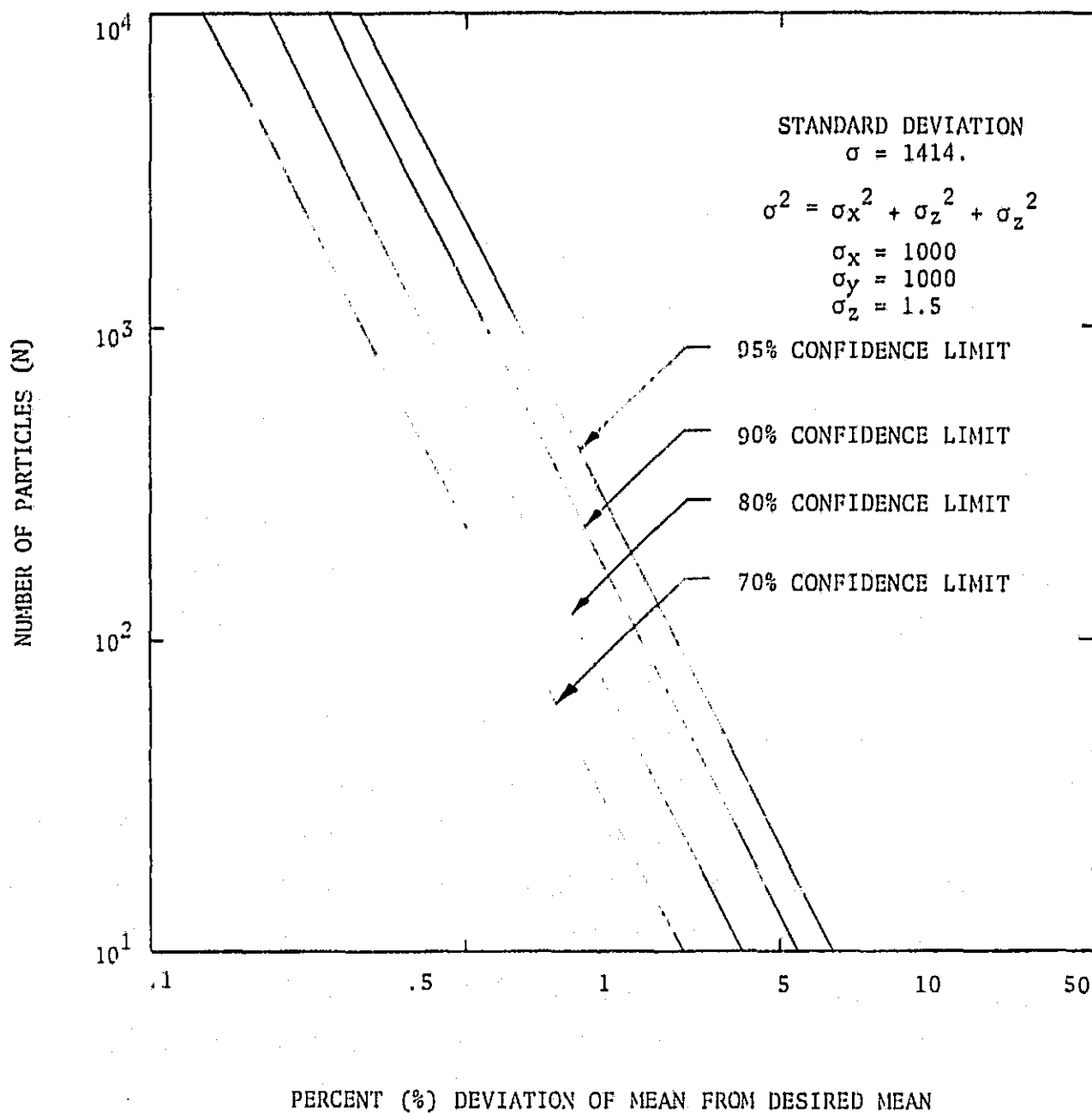


Figure 8.- Number of Particles vs. Percent Deviation of Mean for Varying Confidence Limits Assuming Fixed Mean ($\mu = 5000$) and Standard Deviation ($\sigma = 1414$).

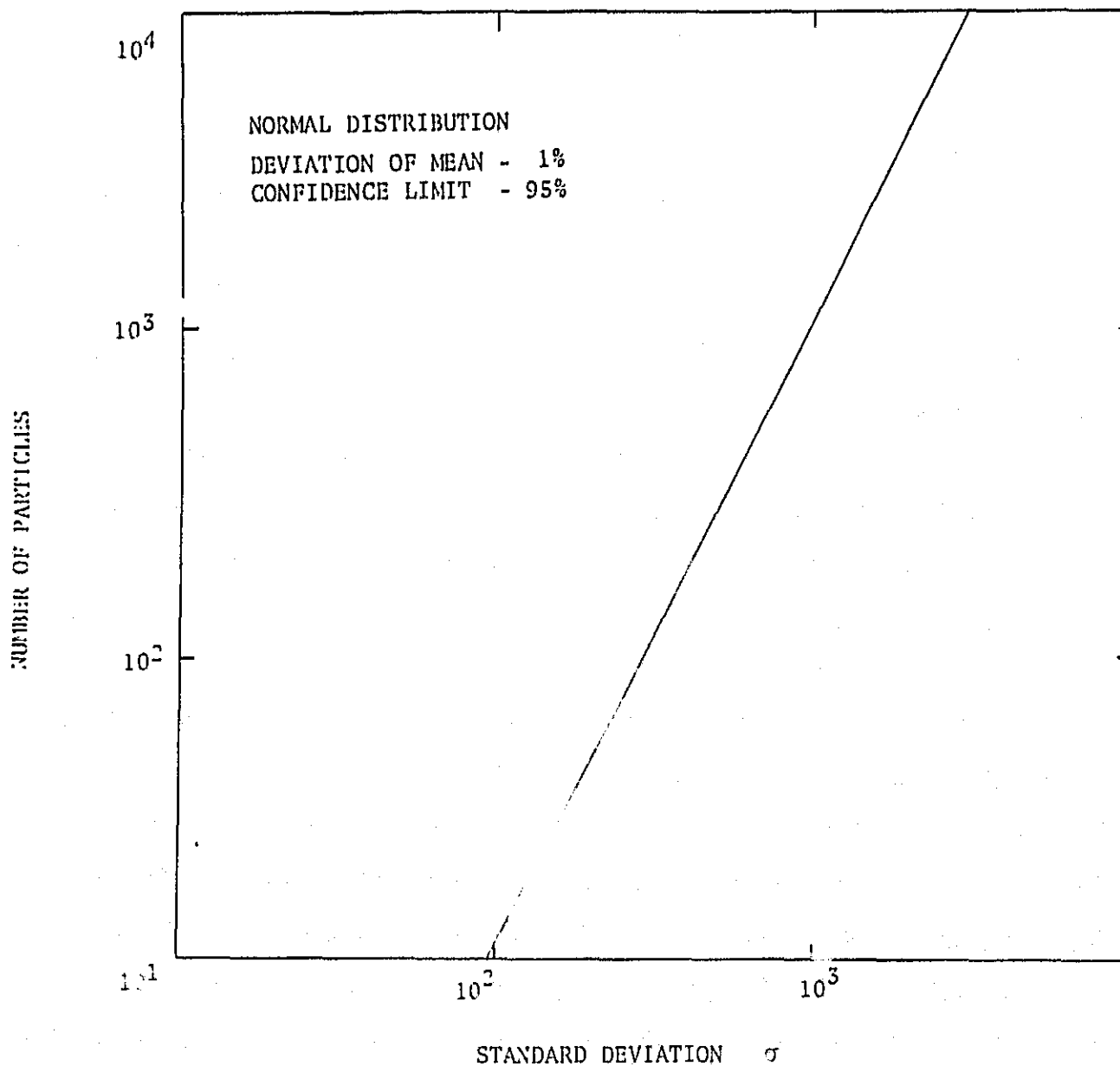


Figure 9.- Influence of Variation in Standard Deviation of Number of Particles for a Given Deviation of the Mean and Confidence Limit.

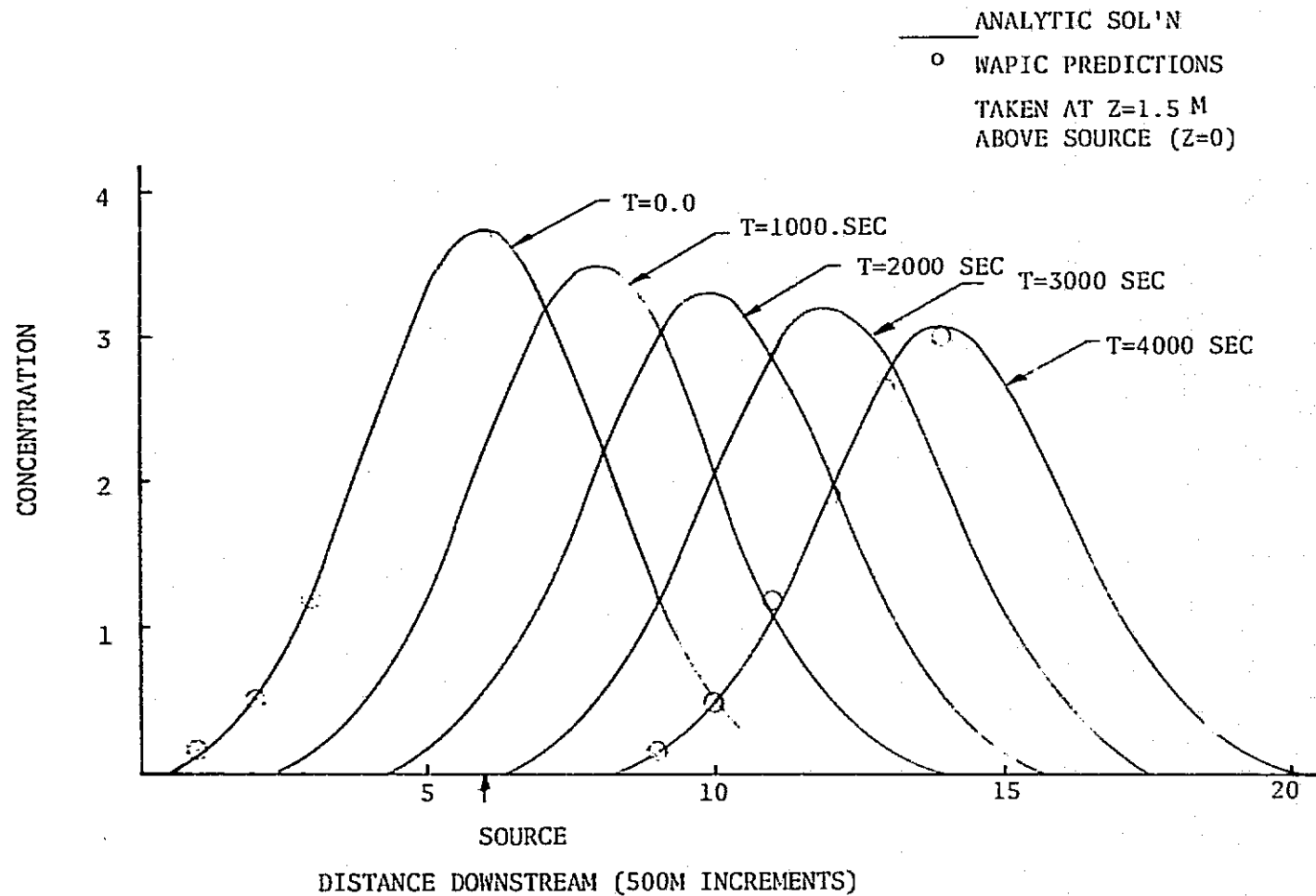


Figure 10.- Concentration vs. Horizontal Distance at Time Increments 0., 1000., 2000., 3000. and 4000. For Instantaneous PT. Release in a Uniform Advection Field.

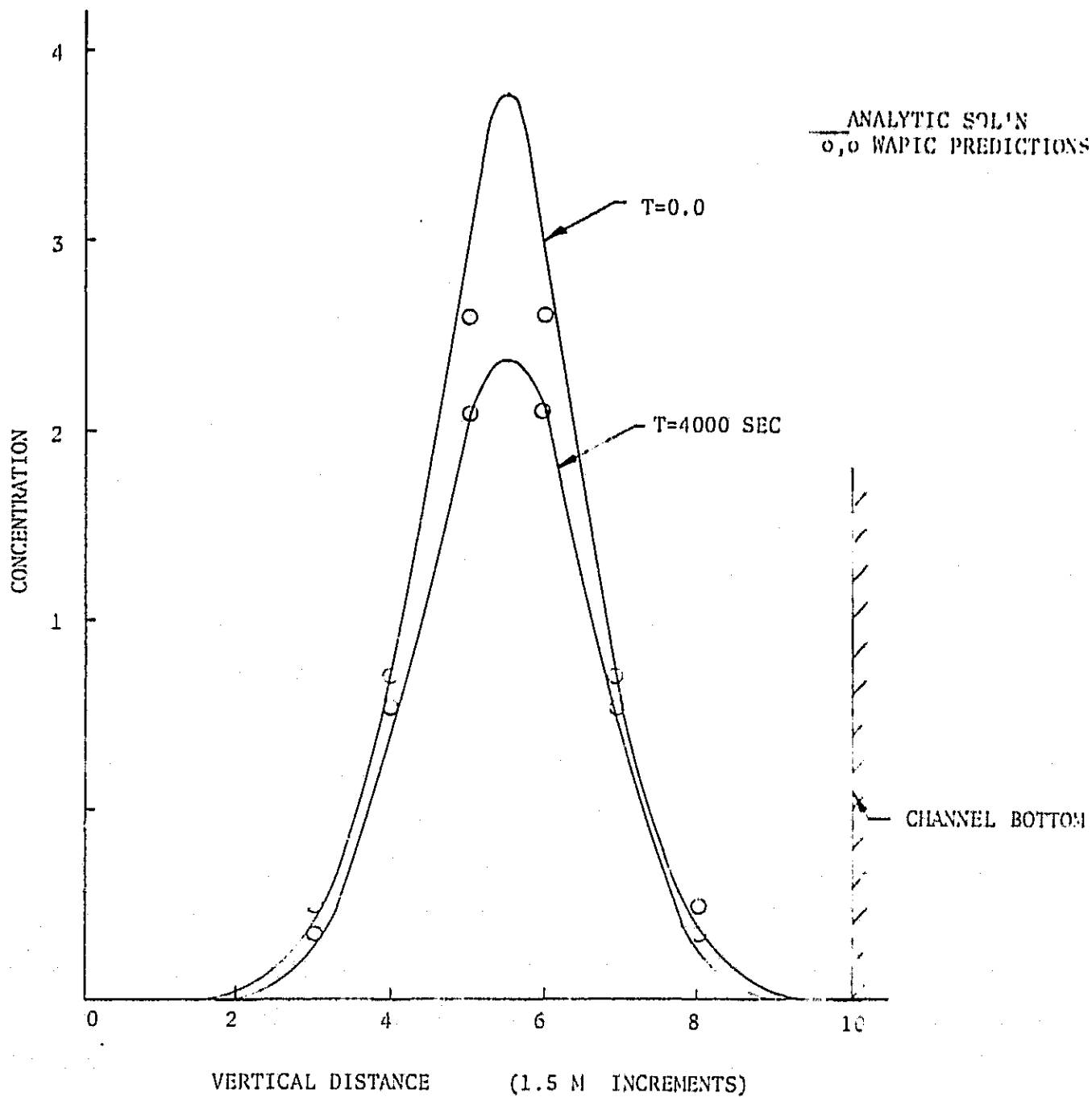


Figure 11.- Concentration vs. Vertical Distance at Time Increments 0 and 4000 Sec. for an Instantaneous Point Release in a Uniform Advection Field